AD-A153 401 CONFORMATIONAL AND MECHANICAL PROPERTIES AT HIGH STRAIN RATES(U) CALIFORNIA UNIV DAVIS W G HOOVER 01 MAR 85 ARO-18611.7-EG DAAG29-82-K-0022 1/1

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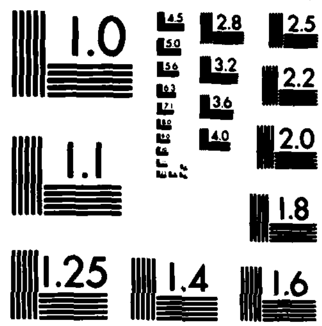

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REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER ARO 18611.7-EG	2. GOVT ACCESSION NO. N/A	3. RECIPIENT'S CATALOG NUMBER N/A
4. TITLE (and Subtitle) Conformational and Mechanical Properties at High Strain Rates		5. TYPE OF REPORT & PERIOD COVERED 7 Dec 81 - 30 Apr 85 Final Report
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) William G. Hoover		8. CONTRACT OR GRANT NUMBER(s) DAAG29-82-K-0022
9. PERFORMING ORGANIZATION NAME AND ADDRESS University of California, Davis		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS U. S. Army Research Office Post Office Box 12211 Research Triangle Park, NC 27709		12. REPORT DATE Mar 85
		13. NUMBER OF PAGES 5
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		15. SECURITY CLASS. (of this report) Unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

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17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

NA

18. SUPPLEMENTARY NOTES

The view, opinions, and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy, or decision, unless so designated by other documentation.

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Mechanical Properties
Strain Rates
Plastic Flow
Plasticity
Powder Compaction
Fracture Properties

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

We have developed several powerful means of studying steady flows far from equilibrium. Gauss' Principle (minimizing the forces of constraint) was found to be useful for most problems, but leads to (small, 10%) errors when applied to heat flow simulations.

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20. ABSTRACT CONTINUED:

~~We have~~ discovered were corresponding-states relations for the rate-dependent viscosity and flux-dependent heat conductivity which are useful in making macroscopic constitutive-equation estimates. Additional keywords: mechanical properties; plastic flow; plasticity; powder compaction; fracture properties; Army research

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1 March 1985

Final Report to
United States Army Research Office
Research Triangle Park, North Carolina

Project Title: Conformational and Mechanical Properties at High Strain Rates

Period Covered by Report: 7 Dec 81 - 30 Apr 85

Grant: DAAG29-82-K-0022

Proposal Number: 18611-EG

Scientific Personnel Supported: William G. Hoover, Principal Investigator
J. Andrew Combs
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Submitted by: William G. Hoover

Problem Studied

As stated in our proposal of 2 April 1981, "Conformational and Mechanical Properites at High Strain Rates," fundamental knowlege of high-speed deformation is very limited. We have provided new insights both on the microscopic atomistic level and at the macroscopic level of constitutive modelling.

During our 42-month study we have analyzed the plastic flow of solids (1, 2, 3) reviewed and developed new simulation methods for studying mass, momentum, and energy flows (4, 5, 6, 7, 8, 9). We have considered the macroscopic aspects of plasticity, fracture, and powder compaction (10, 11, 12). We have begun an extension of these ideas to molecular systems (13) and have considered the technical aspects of some simple problems in elasticity (14, 15). We have most recently studied heat flow simulation in fluids and solids (16).

Summary of Results

We have developed several powerful means of studying steady flows far from equilibrium. Gauss' Principle (minimizing the forces of constraint) was found to be useful for most problems, but leads to (small, 10%) errors when applied to heat flow simulations.

We have discovered corresponding-states relations for the rate-dependent viscosity and flux-dependent heat conductivity which are useful in making macroscopic constitutive-equation estimates.

We have stimulated considerable interest in this area through a series of review articles and through participation in and organization of several international meetings and schools* covering these areas.

*National Bureau of Standards at Boulder (1982)
Orsay CECAM Workshops at Orsay (1983-5)
Euratom Course at Ispra (1984)
Enrico Fermi School of Physics at Varenna (1985)

Related Publications

1. Hoover, W. G., A. J. C. Ladd, and B. Moran. High-Strain-Rate Plastic Flow Studied via Nonequilibrium Molecular Dynamics. Physical Review Letters 48:1818-1820.

2. Ladd, A. J. C., and W. G. Hoover. Energy and entropy of interacting dislocations. Physical Review B 26:5469-5479.

3. Ladd, A. J. C., and W. G. Hoover. Plastic flow in close-packed crystals via nonequilibrium molecular dynamics. Physical Review B 28:1756-1762.

4. Hoover, W. G. Atomistic Nonequilibrium Computer Simulations. Physica 118A:111-122.

5. Evans, D. J., W. G. Hoover, B. H. Failor, B. Moran, and A. J. C. Ladd. Nonequilibrium molecular dynamics via Gauss's principle of least constraint. Physical Review A 28:1-6.

6. Hoover, W. G. Nonequilibrium Molecular Dynamics. Annual Reviews of Physical Chemistry 34:103-127.

7. Hoover, W. G., A. J. C. Ladd, and V. N. Hoover. Historical Development and Recent Applications of Molecular Dynamics Simulation, p. 29-46. In J. M. Haile and G. A. Mansoori (Eds.), Molecular-Based Study of Fluids, American Chemical Society, Washington, D.C.

8. Hoover, W. G. Computer simulation of many-body dynamics. Physics Today, January:44-50.

9. Hoover, W. G. Canonical Dynamics. Equilibrium Phase-Space Distributions. Physical Review A.

10. Hoover, W. G. Simulation of Brittle Fracture Via Molecular Dynamics. Ispra Courses Proceedings Series, Ispra, Italy. 1984.

11. Hoover, W. G. Flow and Plasticity Via Nonequilibrium Molecular Dynamics. Ispra Courses Proceedings Series, Ispra, Italy. 1984.

12. Hoover, W. G. Dynamic Powder Compaction. Ispra Courses Proceedings Series, Ispra, Italy. 1984.

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16. Hoover, W. G., B. Moran, and J. M. Haile. Homogeneous Periodic Heat Flow via Nonequilibrium Molecular Dynamics. Journal of Statistical Physics 37:109-121.

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